What is claimed is:

1. A method for segregating compounds by ionization polarity for use in polarity sensitive analysis thereof, said method comprising the steps of:

a) selecting a data base of a statistically significant group of compounds and determining the polarization, positive or negative, at which each of said compounds is ionized;

b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at positive polarity and to determine structural characteristics common to a majority of compounds which ionize at negative polarity, as polarization determinants;

c) sequentially arranging the polarization determinants in classification trees according to percentage determination of one of said negative or positive polarization;

d) applying the polarization determinants in one of said classification trees in classifying a new compound for a predicted polarization of positive or negative at which said compound is ionized;

e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and

f) separately analyzing the segregated compounds with the respective predicted polarities with an analysis instrument operable in different modes depending on ionization polarity.

2. The method of claim 1, wherein said analysis instrument is a mass spectrometer.

3. The method of claim 2, wherein a polarization determinant is the presence of an OH group.

4. The method of claim 2, wherein a polarization determinant is one of the presence of more than two oxygen atoms and the presence of less than two oxygen atoms.

5. The method of claim 4, wherein the presence of more than two oxygen atoms or the presence of less than two oxygen atoms is a determinant, if an OH group is present.

6. The method of claim 5, wherein, in the absence of an OH group, the presence or absence of CH_2QCH_2 groups, where Q is neither C or H, is a discriminator of polarity.